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Supplementary Information

Synthesis of new C-5-triazolyl-functionalized thymidine analogs and their ability to engage in aromatic stacking in DNA:DNA and DNA:RNA duplexes

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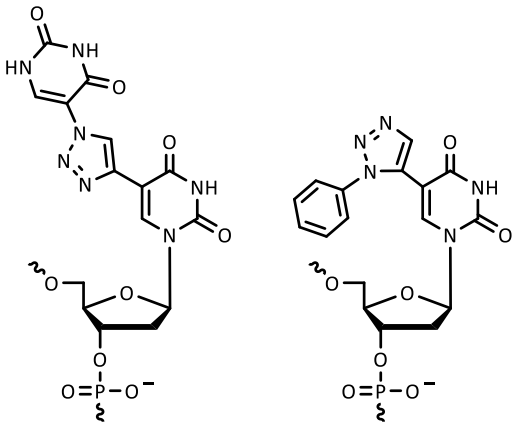
A. MALDI of oligonucleotides

Table A.1. Calculated and found *m*/*z* values for the synthesized oligonucleotides.

Sequence	calcd. mass	found mass‡
5′-dGTG T**Y**T TGC	2898.8	2897.9
5′-dGTG T**YY** TGC	3961.8	3061.8
5′-dGTG **YYY** TGC	3224.8	3224.5
5′-dGTG **YYY Y**GC	3387.8	3387.5
5′-dGTG T**Z**T TGC	2865.0	2867.2
5′-dGTG T**ZZ** TGC	2994.0	2992.3
5′-dGTG **ZZZ** TGC	3123.0	3122.2

‡Mass spectra of the oligonucleotides recorded on a quadrupole MALDI-TOF mass spectrometry instrument in ES^+ mode.



Y Z

B. Selected NMR spectra

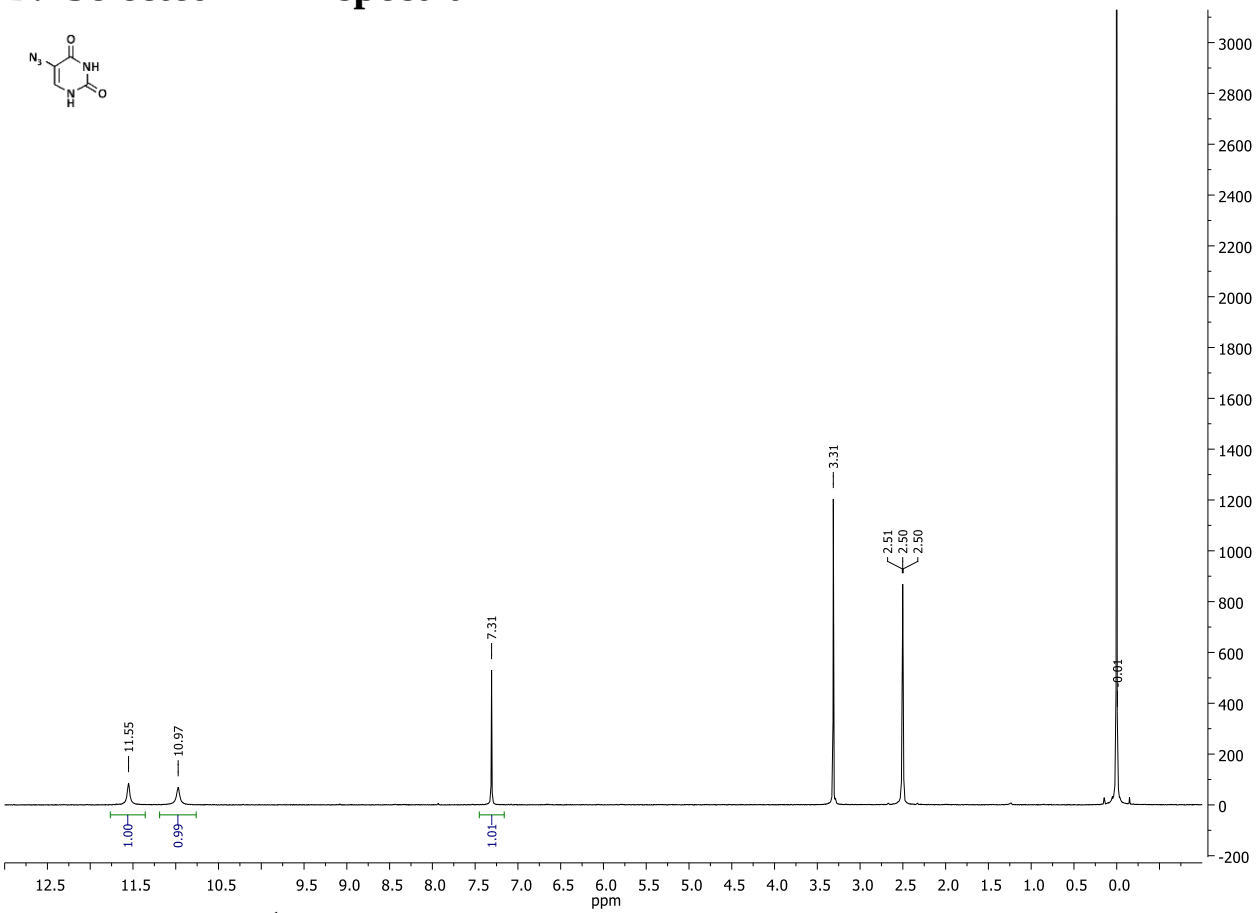


Figure A.1. 400 MHz ^{1}H NMR spectrum of 5-azidouracil in DMSO-d_6.

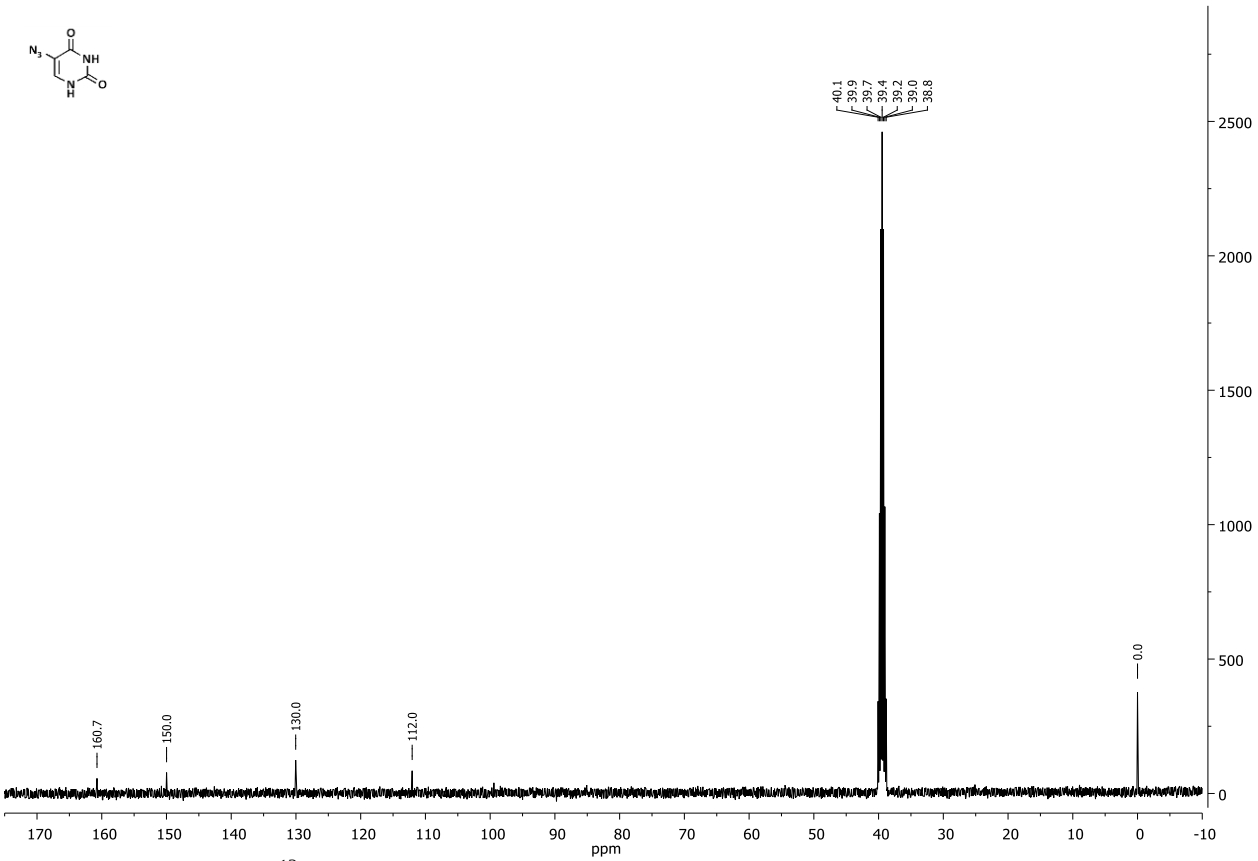


Figure A.2. 101 MHz ^{13}C NMR spectrum of 5-azidouracil in DMSO-d_6.

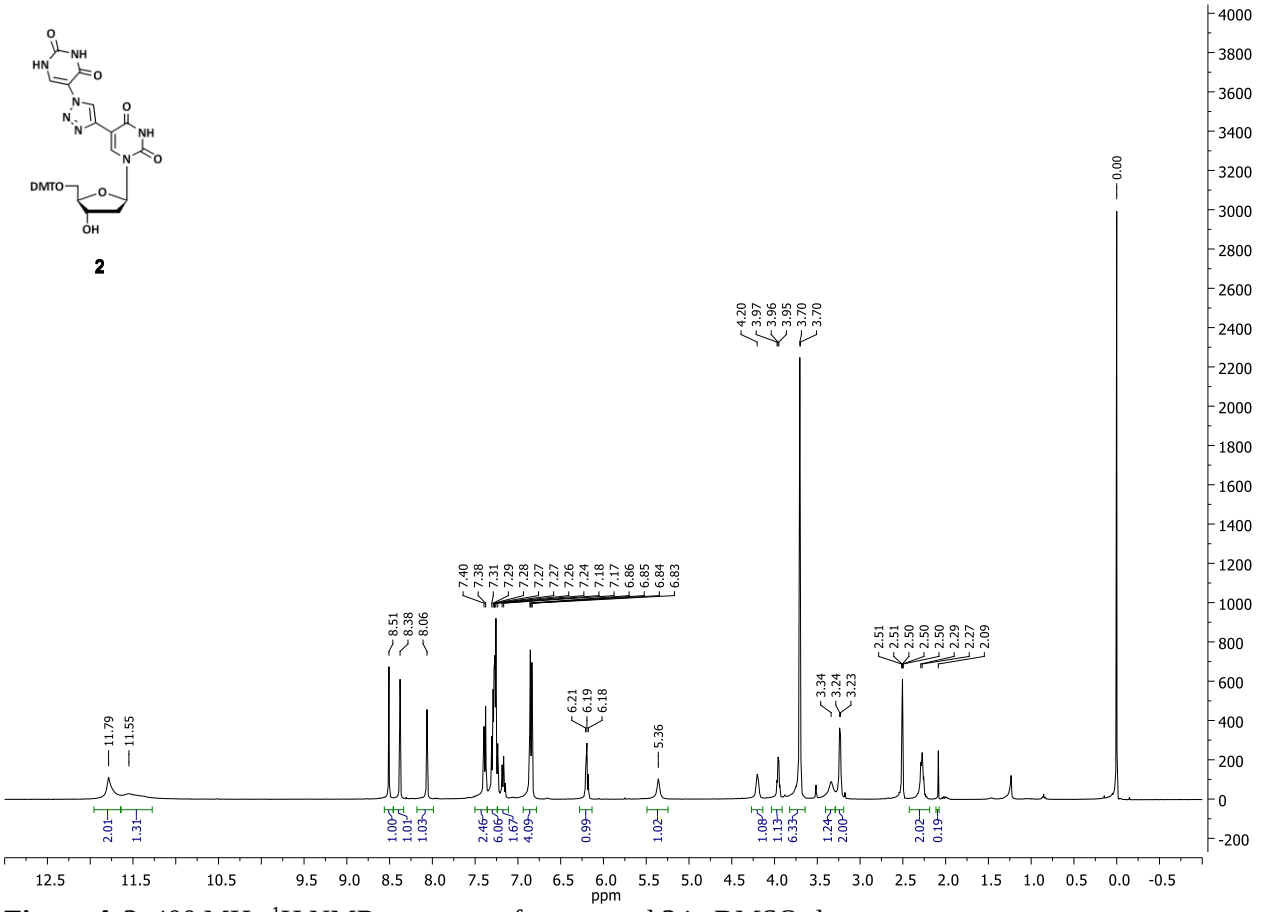


Figure A.3. 400 MHz ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

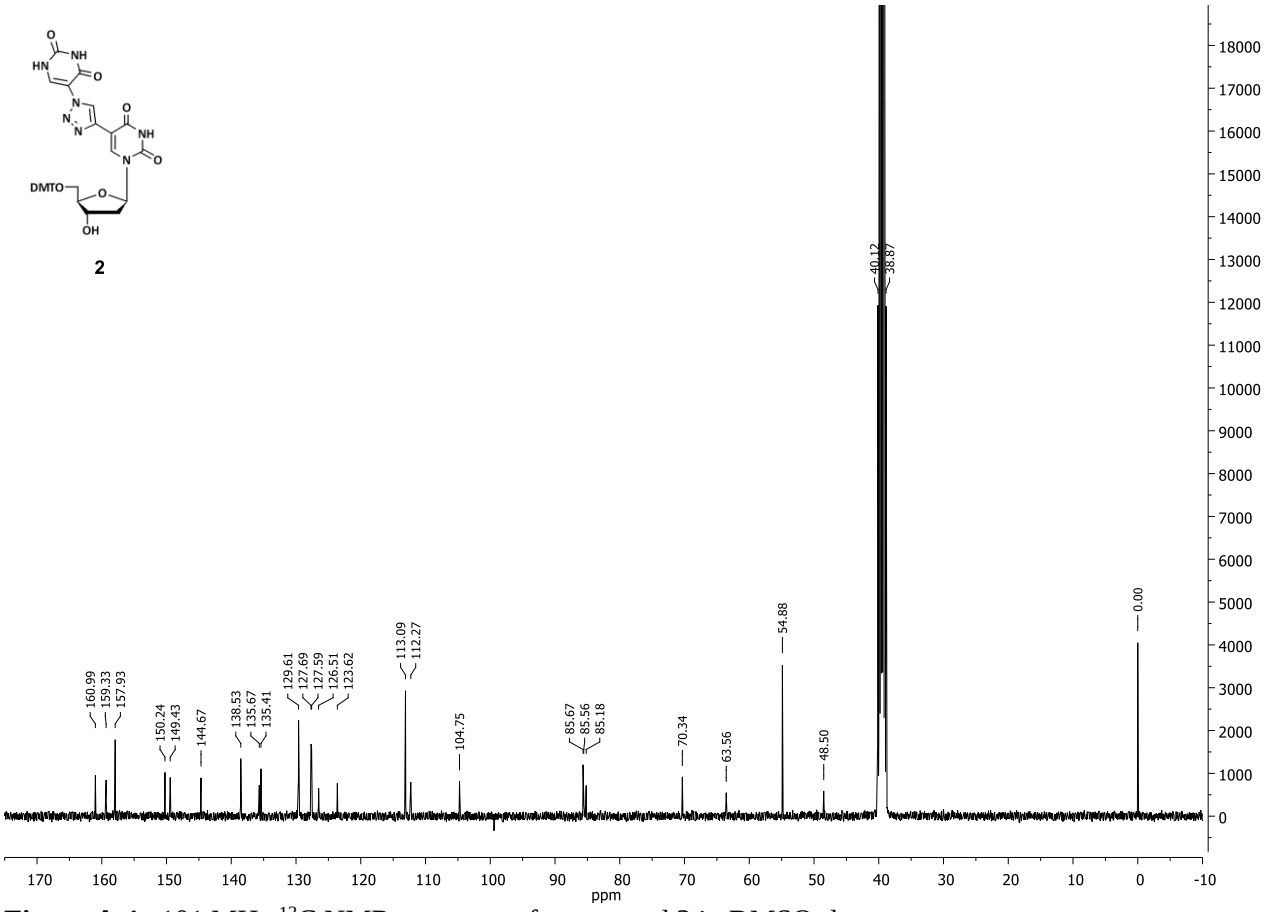


Figure A.4. 101 MHz ^{13}C NMR spectrum of compound **2** in DMSO-d_6.

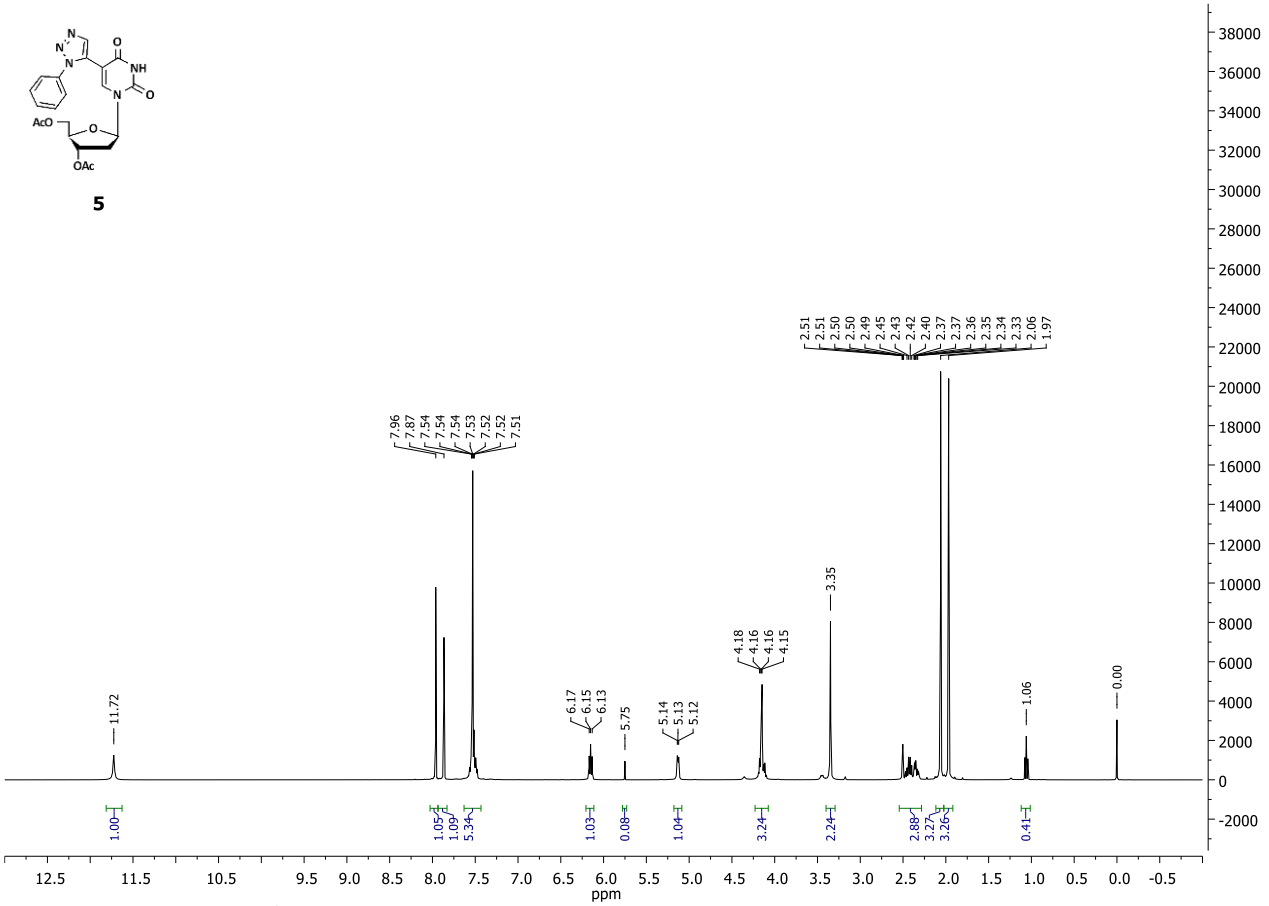


Figure A.5. 400 MHz ^{1}H NMR spectrum of compound **5** in DMSO-d_6.

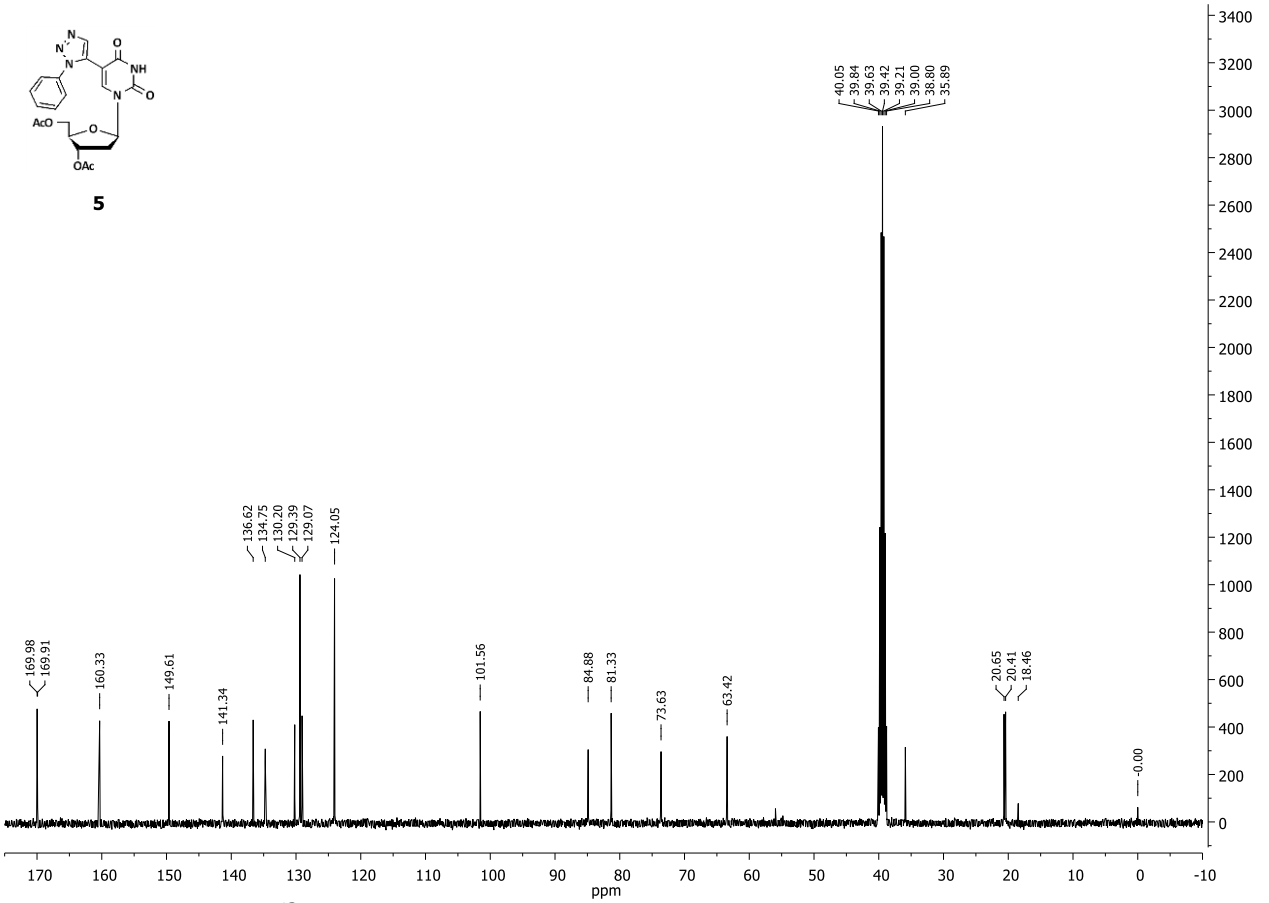


Figure A.6. 101 MHz ^{13}C NMR spectrum of compound **5** in DMSO-d_6.

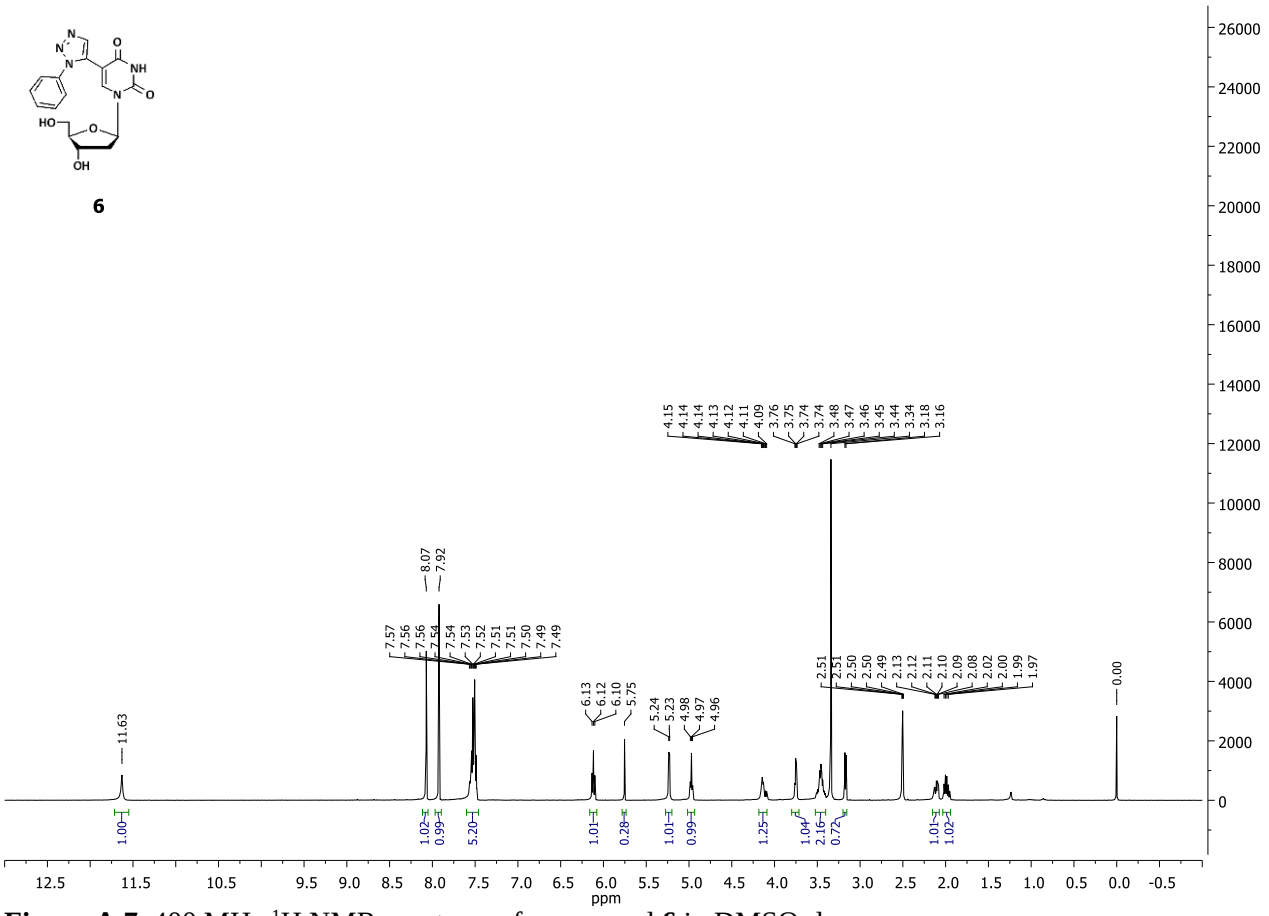


Figure A.7. 400 MHz ^{1}H NMR spectrum of compound **6** in DMSO-d_6.

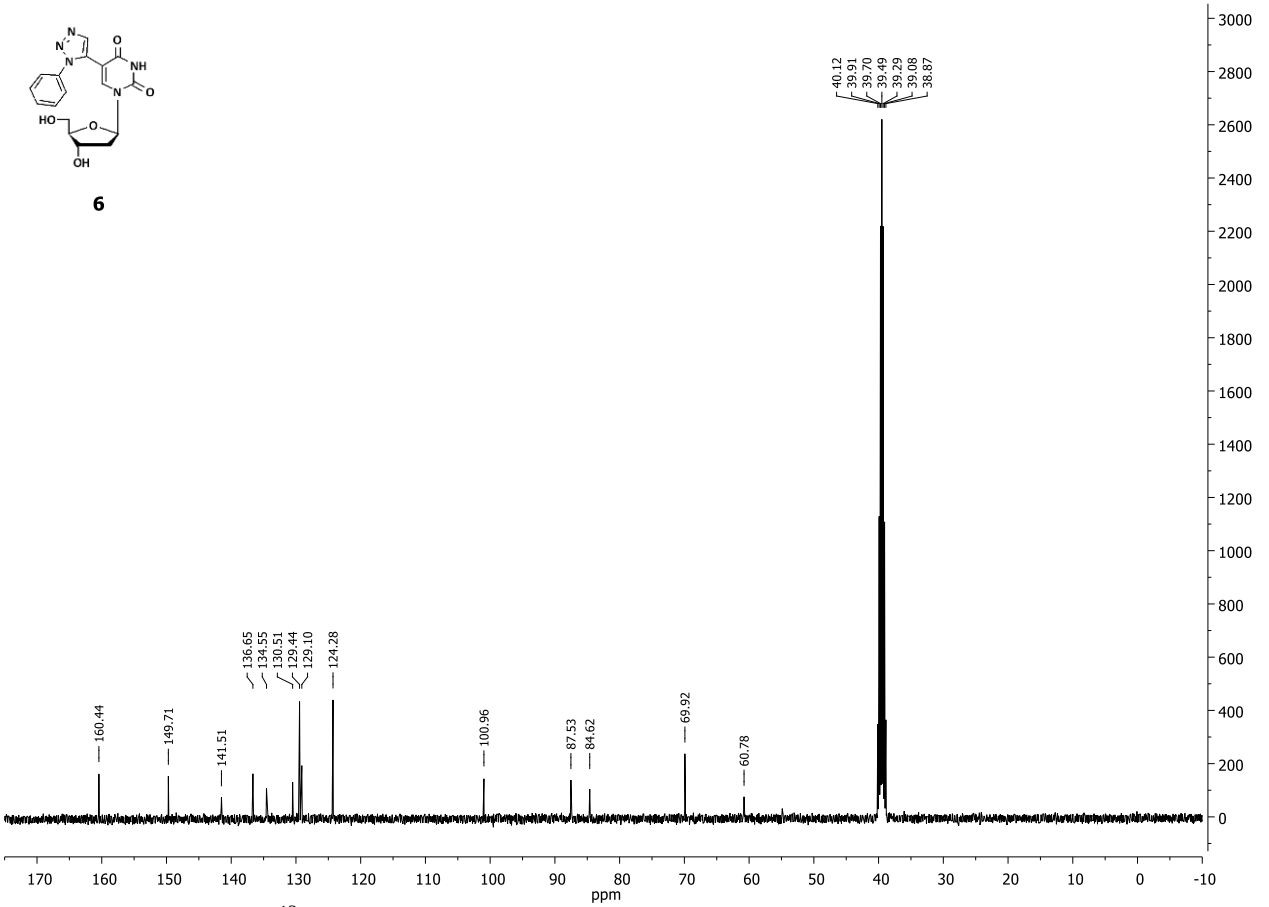


Figure A.8. 101 MHz ^{13}C NMR spectrum of compound **6** in DMSO-d_6.

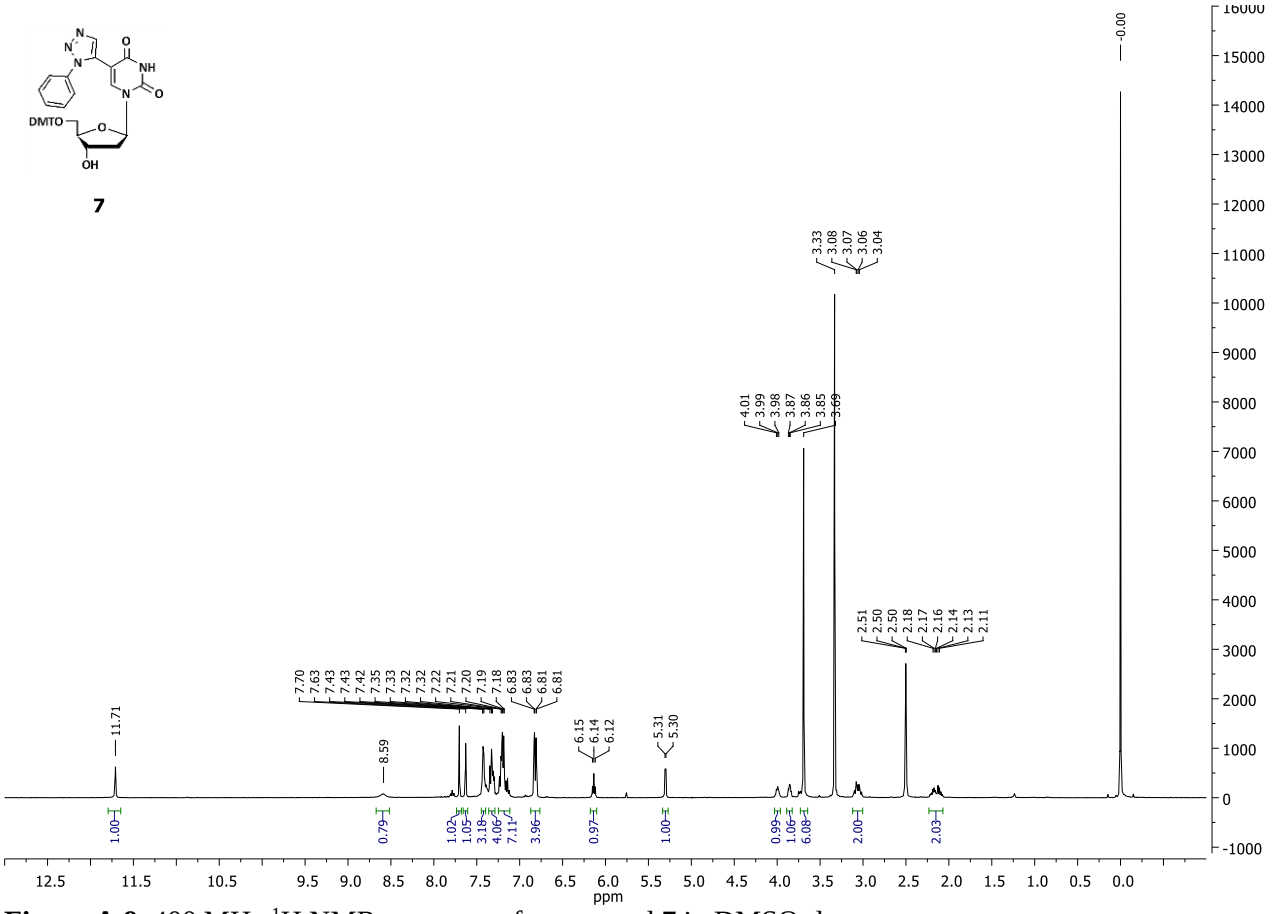


Figure A.9. 400 MHz ^{1}H NMR spectrum of compound **7** in DMSO-d$_6$.

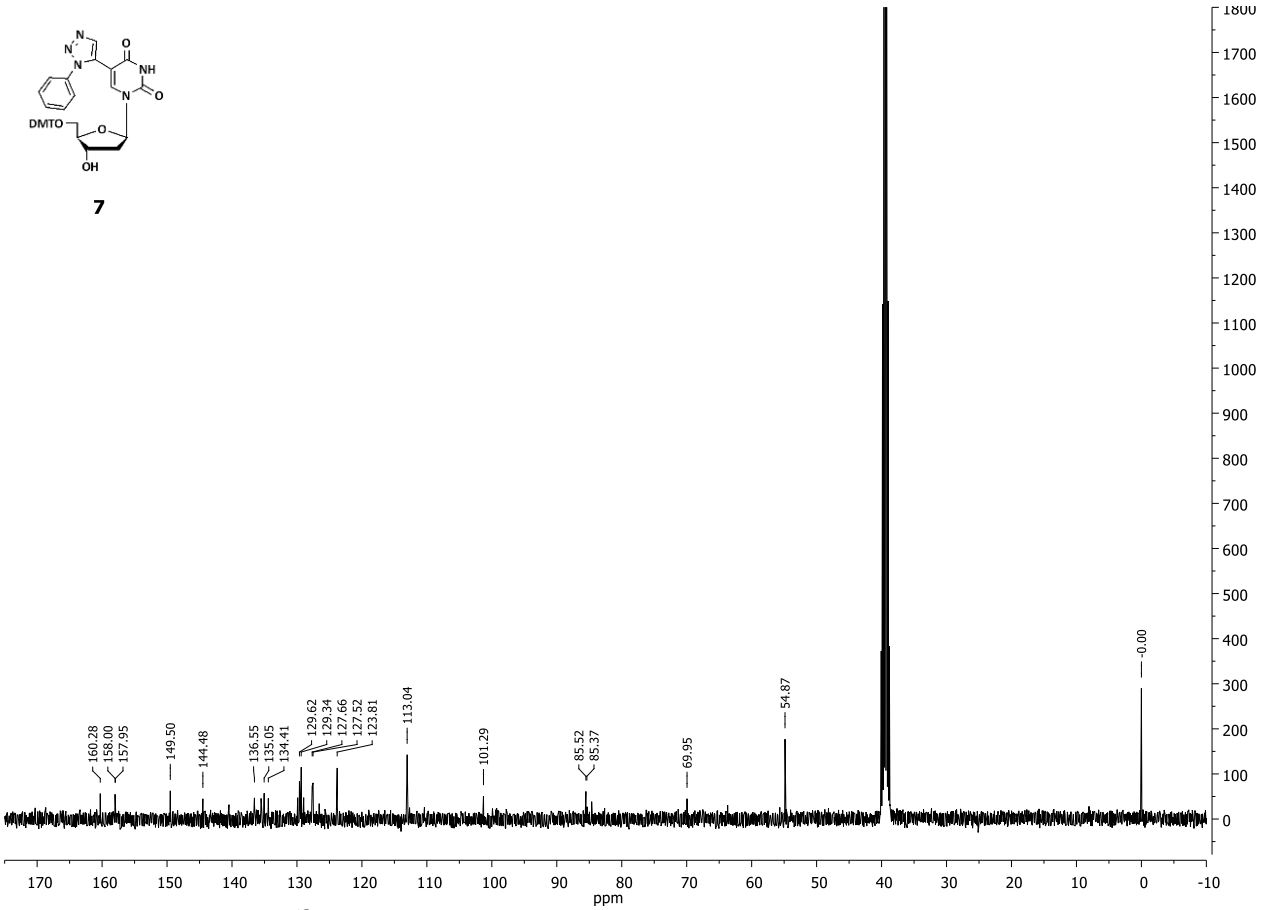


Figure A.10. 101 MHz ^{13}C NMR spectrum of compound **7** in DMSO-d$_6$.

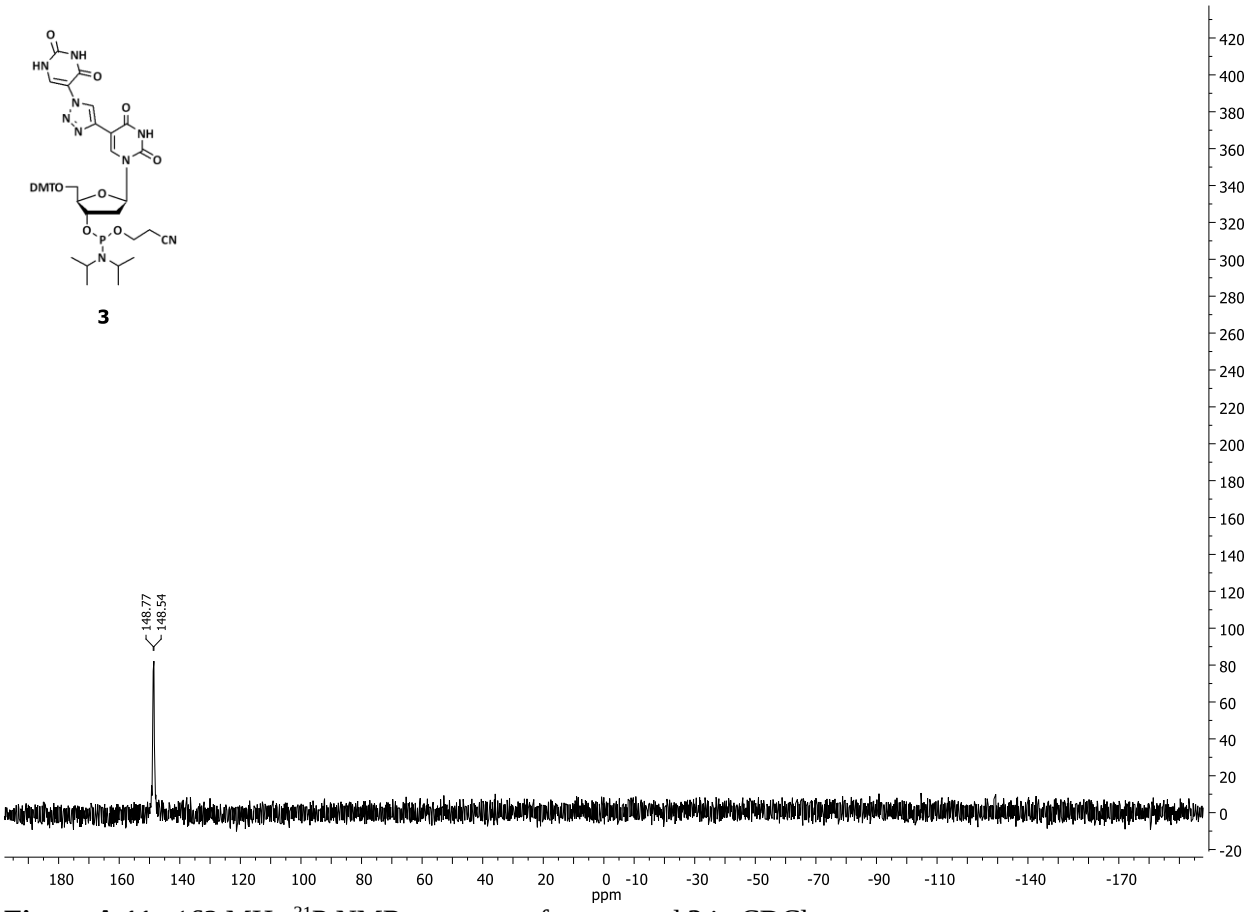


Figure A.11. 162 MHz ^{31}P NMR spectrum of compound **3** in $CDCl_3$.

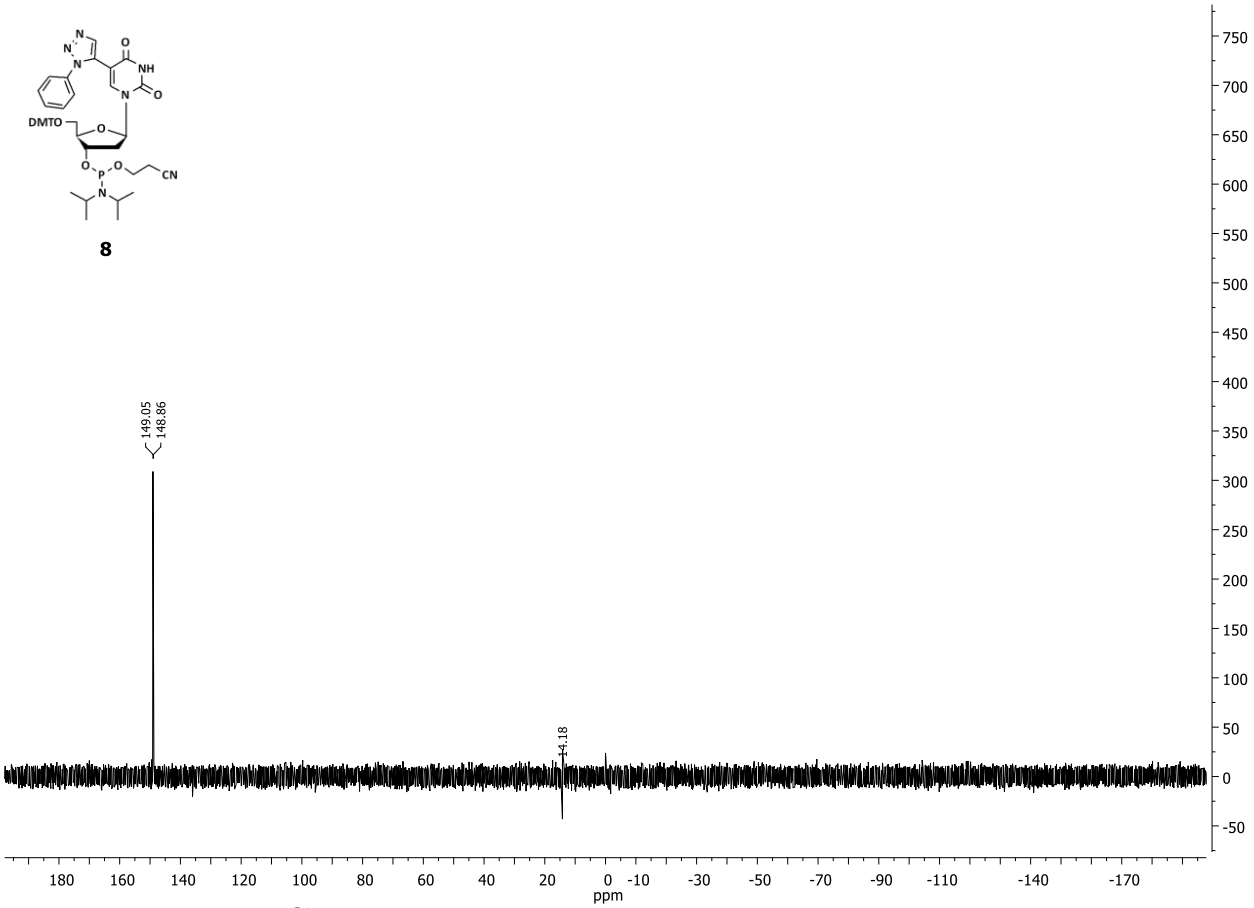


Figure A.12. 162 MHz ^{31}P NMR spectrum of compound **8** in $CDCl_3$.